

Orthogonality criterion for banishing hydrino states from standard quantum mechanics

Antonio S. de Castro

Universidade de Coimbra
Centro de Física Computacional
P-3004-516 Coimbra - Portugal
and
UNESP - Campus de Guaratinguetá
Departamento de Física e Química
12516-410 Guaratinguetá SP - Brasil

Electronic mail: castro@pesquisador.cnpq.br

Abstract

Orthogonality criterion is used to shown in a very simple and general way that anomalous bound-state solutions for the Coulomb potential (hydrino states) do not exist as bona fide solutions of the Schrödinger, Klein-Gordon and Dirac equations.

An alleged tightly-bound state of hydrogen with strong singularity of the eigenfunction at the origin (called a hydrino state) has received considerable attention in the literature [1]. The order of magnitude of the atomic size (Bohr radius) as well as the energy of the hydrogen atom in its ground state just derived from the Heisenberg uncertainty principle, even in a relativistic framework, should be enough to disqualify hydrino states. However, in a recent Letter, Dombey [1] rejects the solution of the three-dimensional Klein-Gordon equation, previously derived by Naudts [2], as well as the solution of the two-dimensional Dirac equation, by resorting to a few fair arguments. In addition, Dombey presents a solid argument founded on the Hermiticity of the Hamiltonian for the Klein-Gordon case and a suggestion of similar treatment for the three-dimensional Dirac case. In the wake of Dombey's suggestion, this Letter presents such a general criterion for banishing hydrino states in the context of the standard quantum mechanics.

The time-independent Schrödinger equation

$$-\frac{\hbar^2}{2M}\nabla^2\psi + V\psi = E\psi \quad (1)$$

and the time-independent Klein-Gordon equation

$$-\hbar^2c^2\nabla^2\psi + M^2c^4\psi = (E - V)^2\psi \quad (2)$$

with spherically symmetric potentials admit eigenfunctions in the form

$$\psi = \frac{u_k(r)}{r} Y_{lm}(\theta, \phi) \quad (3)$$

where k denotes the principal quantum number plus other possible quantum numbers, u_k is a square-integrable function ($\int_0^\infty dr |u_k|^2 = 1$) and Y_l^m are the orthonormalized spherical harmonics ($\int d\Omega Y_{lm}^* Y_{l\tilde{m}} = \delta_{ll} \delta_{m\tilde{m}}$), with $l = 0, 1, 2, \dots$ and $m = -l, -l+1, \dots, l$, in such a way that

$$H_{\text{eff}} u_k = (E_{\text{eff}})_k u_k \quad (4)$$

with

$$H_{\text{eff}} = \begin{cases} -\frac{\hbar^2}{2M} \frac{d^2}{dr^2} + V + \frac{\hbar^2 l(l+1)}{2Mr^2} & \text{for the Schrödinger equation} \\ -\frac{\hbar^2}{2M} \frac{d^2}{dr^2} + \frac{E}{Mc^2} V - \frac{V^2}{2Mc^2} + \frac{\hbar^2 l(l+1)}{2Mr^2} & \text{for the Klein-Gordon equation} \end{cases} \quad (5)$$

and

$$E_{\text{eff}} = \begin{cases} E & \text{for the Schrödinger equation} \\ \frac{E^2 - M^2 c^4}{2Mc^2} & \text{for the Klein-Gordon equation} \end{cases} \quad (6)$$

Meanwhile, the time-independent Dirac equation is

$$H\psi_k = E_k\psi_k, \quad H = \vec{\alpha} \cdot \vec{p} + \beta Mc^2 + V \quad (7)$$

where α_i and β in the standard (or Dirac-Pauli) representation are given by the 2×2 block matrix form

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad i = 1, 2, 3 \quad (8)$$

and σ_i are the 2×2 Pauli matrices. Its eigenfunction has a spinorial structure given by [3]

$$\psi = \frac{1}{r} \begin{pmatrix} i f_k(r) \mathcal{Y}_{jm_j}^\kappa(\theta, \phi) \\ g_k(r) \mathcal{Y}_{jm_j}^{-\kappa}(\theta, \phi) \end{pmatrix} \quad (9)$$

where $\kappa = \mp(j + 1/2)$, with the minus sign for aligned spin ($j = l + 1/2$) and the plus sign for unaligned spin ($j = l - 1/2$). Here, $\mathcal{Y}_{jm_j}^\kappa$ (with $j = 1/2, 3/2, 5/2, \dots$ and $m_j = -j, -j + 1, \dots, j$) are the orthonormalized spinor spherical harmonics resulting from the coupling of two-dimensional spinors to the eigenstates of orbital angular momentum. The normalization of the Dirac spinor ($\int_0^\infty dr (|f_k|^2 + |g_k|^2) = 1$) requires that f_k and g_k are square-integrable functions. Using the identity $\vec{\sigma} \cdot \vec{\nabla} = \vec{\sigma} \cdot \hat{r} \frac{\partial}{\partial r} - \frac{\vec{\sigma} \cdot \hat{r} \vec{\sigma} \cdot \vec{L}}{\hbar r}$ and the properties $\vec{\sigma} \cdot \hat{r} \mathcal{Y}_{jm_j}^\kappa = -\mathcal{Y}_{jm_j}^{-\kappa}$ and $\vec{\sigma} \cdot \vec{L} \mathcal{Y}_{jm_j}^\kappa = -(\kappa + 1) \mathcal{Y}_{jm_j}^\kappa$, there results that one can write

$$H_{\text{eff}} \Phi_k = E_k \Phi_k \quad (10)$$

where

$$H_{\text{eff}} = \begin{pmatrix} \hbar c \left(\frac{d}{dr} + \frac{\kappa}{r} \right) & V - Mc^2 \\ V + Mc^2 & \hbar c \left(-\frac{d}{dr} + \frac{\kappa}{r} \right) \end{pmatrix}, \quad \Phi_k = \begin{pmatrix} f_k \\ g_k \end{pmatrix} \quad (11)$$

It is instructive to examine the radial solutions in the neighbourhood of the origin for the Coulomb potential $-\hbar c \alpha / r$ (α is the coupling constant) because u , f and g must behave better than $r^{-1/2}$ at the origin in order to guarantee their square integrability. An estimative of the asymptotic behaviour of the radial solutions for small r can be obtained by neglecting the terms of order r^{-n}

compared with the terms of order $r^{-(n+1)}$, where $n = 0, 1, 2$, in the Schrödinger, Klein-Gordon and Dirac differential equations.

As $r \rightarrow 0$ the terms behaving as r^{-2} (r^{-1}) dominate in the Schrödinger case for $l \neq 0$ ($l = 0$) in such a way that

$$r^2 \frac{d^2 u}{dr^2} - l(l+1)u = 0, \quad \text{for } l \neq 0 \quad (12)$$

$$r^2 \frac{d^2 u}{dr^2} + \frac{2Mc\alpha}{\hbar} ru = 0, \quad \text{for } l = 0 \quad (13)$$

Substituting the Frobenius series expansion

$$u = \sum_{n=0}^{\infty} a_n r^{\nu+n}, \quad a_0 \neq 0 \quad (14)$$

into (12) and (13) yields the quadratic indicial equation (obtained when $n = 0$): $\nu(\nu - 1) = l(l + 1)$, which has the solutions $\nu_1 = l + 1$ and $\nu_2 = -l$. It happens that there is no recurrence formula for $l \neq 0$ ($a_n = 0$ for $n \neq 0$) so that the general solution for (12) can be written as $u = A_l r^{l+1} + B_l r^{-l}$. On the other hand, for $l = 0$ the power series expansion fails with $\nu = \nu_2$ because only the first coefficient of the series can be defined. It means that the Frobenius method furnishes only one solution for $l = 0$. A second solution linearly independent of $u_1 = a_0 r + \dots$, the solution related to $\nu = \nu_1$, can be found by writing $u_2 = au_1 \ln(r) + \sum_{n=0}^{\infty} b_n r^{\nu_2+n}$ with $a \neq 0$ and $b_0 \neq 0$. It follows that the general solution for $l = 0$ can be written as $u = A_0 \left(r - \frac{Mc\alpha}{\hbar} r^2 + \dots \right) + B_0 \left(1 - \frac{2Mc\alpha}{\hbar} r \ln(r) + \dots \right)$. The above results imply that only choosing $B_l = B_0 = 0$ gives a behaviour at the origin which can lead to square-integrable solutions. For short, all the normalizable radial solutions (u/r) are regular at the origin and behave as r^l as $r \rightarrow 0$, for all l .

As for the Klein-Gordon case, the terms behaving as r^{-2} , for all values of l , outweighs the other terms in such a manner that one can write

$$r^2 \frac{d^2 u}{dr^2} - [l(l+1) - \alpha^2] u = 0 \quad (15)$$

for small r . The power series expansion (14) gives the indicial equation $\nu(\nu - 1) = l(l + 1) - \alpha^2$ which has the roots

$$\nu_{\pm} = \frac{1}{2} \pm \sqrt{\left(l + \frac{1}{2}\right)^2 - \alpha^2}, \quad \alpha \leq l + \frac{1}{2} \quad (16)$$

The argumentation given below is based on (16) and can be better understood by observing Fig. 1, where ν_+ and ν_- , as a function of α , are plotted on the same grid. The constraint $\nu > -1/2$ which ensures the square integrability of u demands that for $\alpha \leq 1/2$ there are just a S-wave ($l = 0$) solution for $\nu = \nu_-$ although all the values of l are allowed for $\nu = \nu_+$. Since $\nu < 1$ for $\alpha \leq 1/2$, both S-wave solutions, in the sense of u/r , diverge at the origin. As α increases some normalizable solutions diverging at the origin for $\nu = \nu_-$ become possible whereas some normalizable solutions for $\nu = \nu_+$ become divergent. In any case, as the coupling constant takes critical values ($\alpha_c = l_c + 1/2$, $l_c = 0, 1, 2, \dots$) only the solutions for $l > l_c$ are allowed.

In analogy with the solutions in the neighbourhood of the origin of the Schrödinger and Klein-Gordon equations, we look for solutions of the asymptotic Dirac equation

$$r \frac{df}{dr} + \kappa f - \alpha g = 0$$

$$(17)$$

$$r \frac{dg}{dr} - \kappa g + \alpha f = 0$$

in the form of power series

$$f = \sum_{n=0}^{\infty} a_n r^{\nu+n}, \quad a_0 \neq 0$$

$$(18)$$

$$g = \sum_{n=0}^{\infty} b_n r^{\nu+n}, \quad b_0 \neq 0$$

Now the coefficient of r^ν ($n = 0$) gives the system of indicial equations

$$(\nu + \kappa) a_0 - \alpha b_0 = 0$$

$$(19)$$

$$\alpha a_0 + (\nu - \kappa) b_0 = 0$$

and the two possible values of ν :

$$\nu_{\pm} = \pm \sqrt{\kappa^2 - \alpha^2}, \quad \alpha \leq |\kappa|$$

$$(20)$$

Fig. 2 illustrates (20) as a function of the coupling constant for the lowest values of $|\kappa|$. The requirement of normalizability ($\nu > -1/2$) implies that for $\alpha \leq \sqrt{3}/2$

only the positive root is allowed and the radial solutions (f/r and g/r) are found for all the values of $|\kappa|$ ($|\kappa| = 1, 2, 3, \dots$), although the radial solutions with $|\kappa| = 1$ diverge at the origin. The negative root allows divergent radial solutions with $|\kappa| = 1$ for $\sqrt{3}/2 < \alpha \leq 1$. Nevertheless, there are no normalizable solutions with $|\kappa| = 1$ for $\alpha > 1$. Continuing this process, as the coupling constant increases starting with $\alpha = 1$, some normalizable solutions for $\nu = \nu_+$ turn out to be divergent whereas some normalizable solutions diverging at the origin for $\nu = \nu_-$ become possible. As α takes critical values ($\alpha = |\kappa|_c$, $|\kappa|_c = 1, 2, 3, \dots$) only the solutions for $|\kappa| > |\kappa|_c$ are allowed. This means that the radial solutions for the smallest values of $|\kappa|$ become disallowed one after the other as α increases.

In the standard quantum mechanics an observable such as the energy is represented by an Hermitian operator, whose set of eigenfunctions constitutes a basis so that every arbitrary wave function can be expanded in one and only one way in terms of the eigenfunctions. Besides square-integrability, appropriate boundary conditions must be imposed on the eigenfunctions of an eigenvalue problem. Square-integrability requires that the eigenfunction vanishes at the infinity and the boundary condition at the origin for a singular potential, as the Coulomb potential, comes naturally into existence by demanding that the Hamiltonian is Hermitian, viz.

$$\int_0^\infty d\tau \psi_k^* (H\psi_{k'}) = \int_0^\infty d\tau (H\psi_k)^* \psi_{k'} \quad (21)$$

where ψ_k is an eigenfunction corresponding to an eigenvalue E_k . In passing, note that a necessary consequence of Eq. (21) is that the eigenfunctions corresponding to distinct effective eigenvalues are orthogonal. Identifying H_{eff} with H and E_{eff} with E in (21), integrating by parts and recalling the orthonormality of the spherical harmonics, it is easy to show that $u_k(r)$ for the Schrödinger and Klein-Gordon cases must satisfy the following constraint [4]-[5]

$$\lim_{r \rightarrow 0} \left(u_k^* \frac{du_{k'}}{dr} - \frac{du_k^*}{dr} u_{k'} \right) = 0 \quad (22)$$

For the Dirac case, identifying H_{eff} with H in (21), one finds a constraint involving the upper and lower components, namely [4]-[5]

$$\lim_{r \rightarrow 0} (f_k^* g_{k'} - f_{k'}^* g_k) = 0 \quad (23)$$

For the Schrödinger case, the square-integrable solution for u ($u \rightarrow r^{l+1}$ as $r \rightarrow 0$) satisfies (22) and its corresponding radial solution u/r is regular at the

origin.

For the Klein-Gordon case, only the solutions for u less singular than $r^{1/2}$ can satisfy the orthogonality criterion. One sees, then, that the square-integrable solution must behave as r^{ν_+} , as $r \rightarrow 0$, where ν_+ is one of the two possibilities of (16), corresponding to the thick lines in Fig. 1. Therefore, square-integrable solutions of the Klein-Gordon equation satisfying the orthogonality criterion are such that for $\alpha \leq 1/2$ all the values of l are allowed. The $l = 0$ radial solution, in the sense of u/r , has a divergence at the origin. As α increases some regular normalizable solutions become divergent. In any case, as the coupling constant takes critical values ($\alpha_c = l_c + 1/2$, $l_c = 0, 1, 2, \dots$) we are left with the solutions for $l > l_c$.

For the Dirac case, only the regular solutions for f and g can satisfy the orthogonality criterion. This means that the square-integrable solutions must behave at the origin as r^{ν_+} , where ν_+ is the positive square root of (20), corresponding to the thick lines in Fig. 2. Here, square-integrable solutions satisfying the orthogonality criterion are such that, for $\alpha \leq 1$, the radial solutions (f/r and g/r) are found for all the values of $|\kappa|$ ($|\kappa| = 1, 2, 3, \dots$), with the radial solutions with $|\kappa| = 1$ diverging at the origin. Nevertheless, there are no normalizable solutions with $|\kappa| = 1$ for $\alpha > 1$. Continuing this process, as α increases starting with $\alpha = 1$, some solutions turn out to be divergent. As α takes critical values ($\alpha = |\kappa|_c$, $|\kappa|_c = 1, 2, 3, \dots$) only the solutions for $|\kappa| > |\kappa|_c$ are allowed. This means that the radial solutions for the smallest values of $|\kappa|$ become disallowed one after the other as α increases.

In summary, a very simple and general criterion has been presented to reject hydrino states in the context of the standard quantum mechanics. Square integrability is sufficient enough to exclude singular wave functions in the Schrödinger equation, but not in the Klein-Gordon and Dirac ones. For the relativistic equations with the Coulomb potential, singular wave functions are allowed. The orthogonality criterion, though, imposes an additional constraint in such way that the would-be relativistic square-integrable solutions for hydrino states, related to the thin lines in Fig. 1 and Fig. 2, are not acceptable. Therefore, only radial solutions behaving at the origin as $r^{-1/2+\varepsilon}$, with $\varepsilon > 0$, for the Klein-Gordon case, and $r^{-1+\varepsilon}$ for the Dirac case, are physically acceptable solutions.

Acknowledgments

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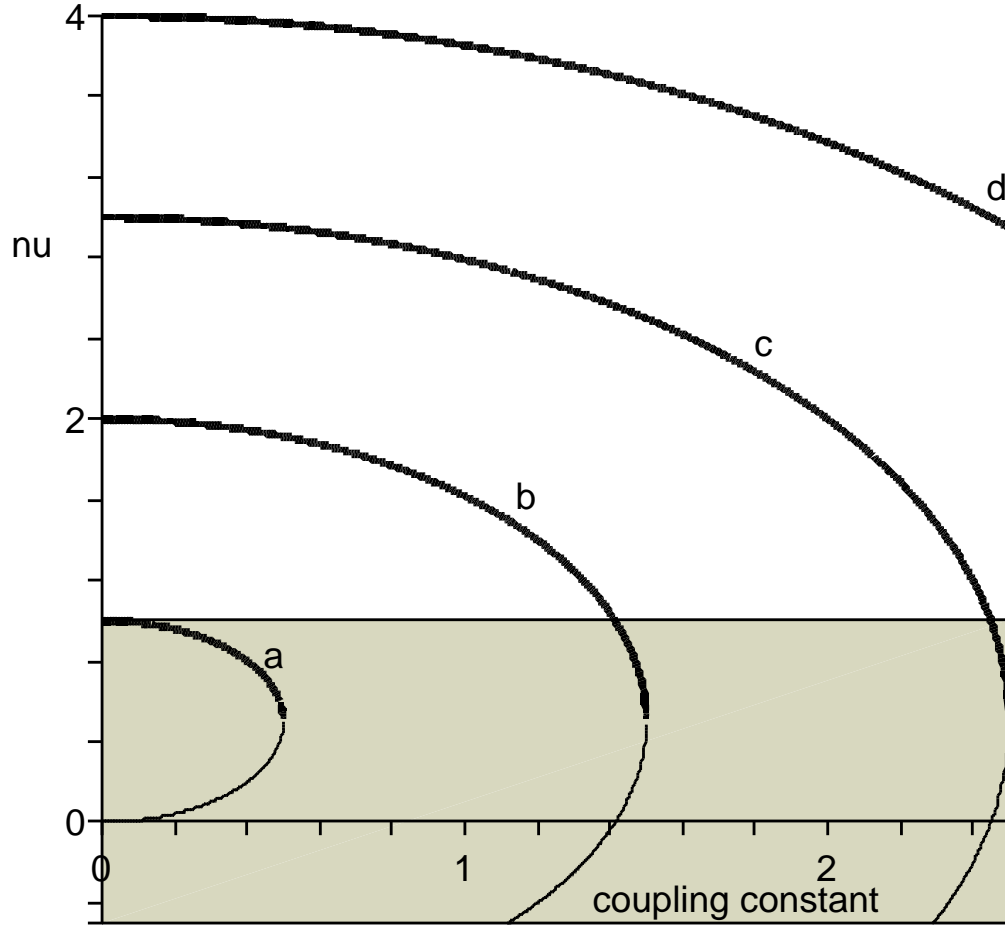


Figure 1: The roots of the indicial equation, ν_+ (thick line) and ν_- (thin line), as a function of the coupling constant for the Klein-Gordon case (a for $l = 0$, b for $l = 1$, c for $l = 2$ and d for $l = 3$). The shaded area represents the zone corresponding to radial solutions diverging at the origin.

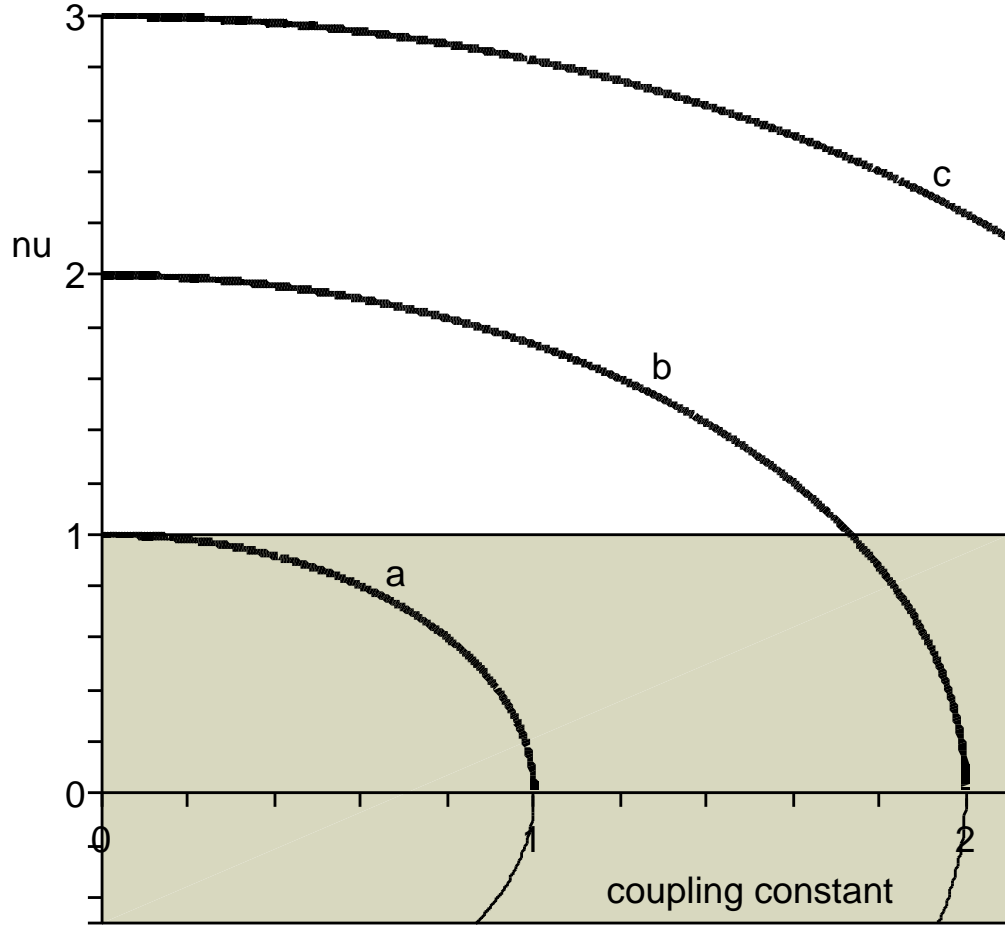


Figure 2: The solutions of the system of indicial equations, ν_+ (thick line) and ν_- (thin line), as a function of the coupling constant for the Dirac case (a for $|\kappa| = 1$, b for $|\kappa| = 2$ and c for $|\kappa| = 3$). The shaded area represents the zone corresponding to radial solutions diverging at the origin.